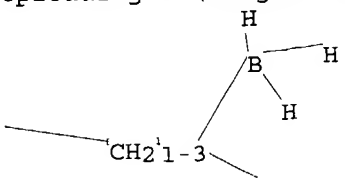
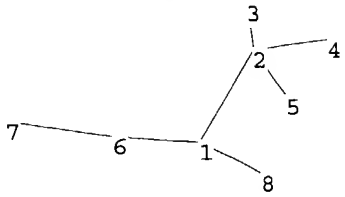
=>
Uploading C:\Program Files\Stnexp\Queries\10625982.str



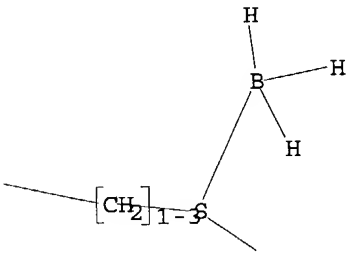


chain nodes :
1 2 3 4 5 6 7 8
chain bonds :
1-2 1-6 1-8 2-3 2-4 2-5 6-7
exact/norm bonds :
1-8
exact bonds :
1-2 1-6 2-3 2-4 2-5 6-7

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 15:18:34 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 174 TO ITERATE

100.0% PROCESSED 174 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 2689 TO 4271
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 full

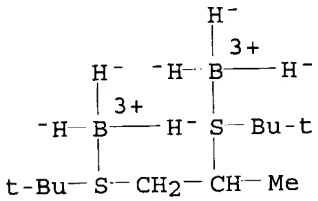
FULL SEARCH INITIATED 15:18:37 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 4043 TO ITERATE

100.0% PROCESSED 4043 ITERATIONS 25 ANSWERS
SEARCH TIME: 00.00.01

L3 25 SEA SSS FUL L1

=> d scan

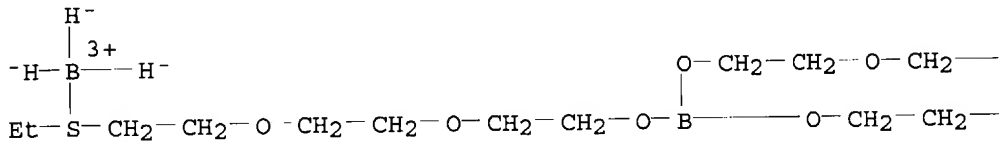
L3 25 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Boron, hexahydro[μ-[2,2'-[(1-methyl-1,2-ethanediyl)bis(thio)]bis[2-methylpropane]-S:S']]di- (9CI)
MF C11 H30 B2 S2
CI CCS



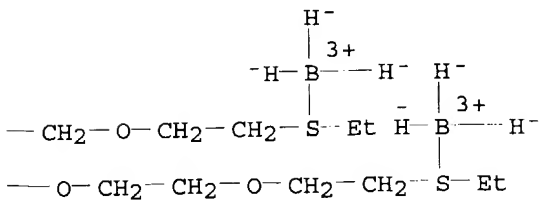
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L3 25 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Boron, nonahydro[μ3-[tris[2-[2-[2-(ethylthio-κS)ethoxy]ethoxy]ethyl] orthoborate]]tri- (9CI)
MF C24 H60 B4 O9 S3
CI CCS

PAGE 1-A

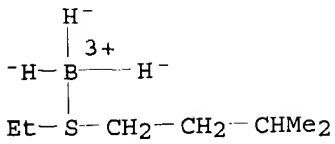


PAGE 1-B

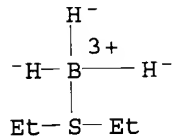


L3 25 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

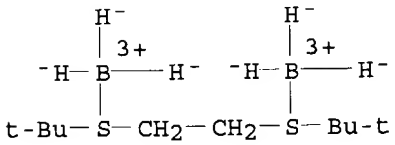
IN Boron, [1-(ethylthio)-3-methylbutane]trihydro-, (T-4)- (9CI)
MF C7 H19 B S
CI CCS



L3 25 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Boron, trihydro[1,1'-thiobis[ethane]]-, (T-4)- (9CI)
MF C4 H13 B S
CI CCS

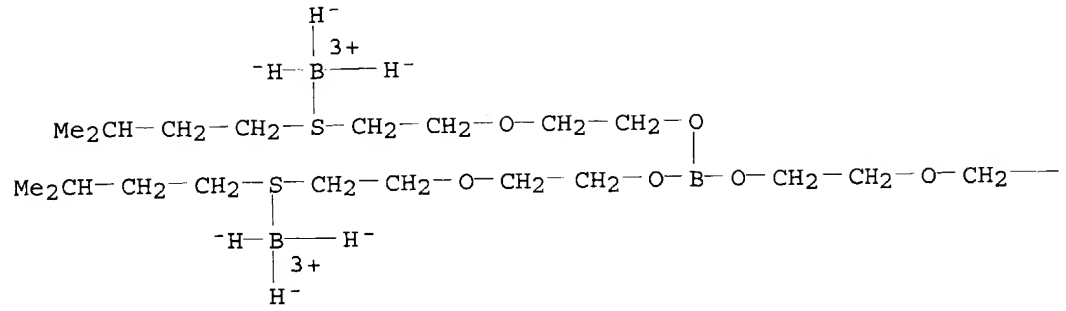


L3 25 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Boron, [μ-[2,2'-[1,2-ethanediylbis(thio-κS)]bis[2-methylpropane]]]hexahydrodi- (9CI)
MF C10 H28 B2 S2
CI CCS

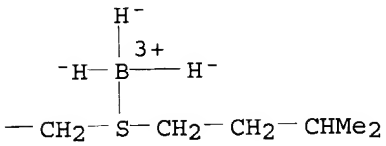


L3 25 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Boron, nonahydro[μ3-[tris[2-[2-[(3-methylbutyl)thio-κS]ethoxy]ethyl] orthoborate]]tri- (9CI)
MF C27 H66 B4 O6 S3
CI CCS

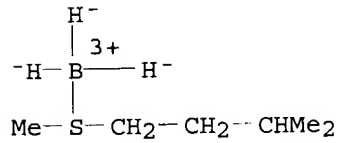
PAGE 1-A



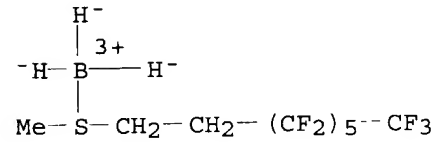
PAGE 1-B



L3 25 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Boron, trihydro[3-methyl-1-(methylthio)butane]-, (T-4)- (9CI)
MF C6 H17 B S
CI CCS

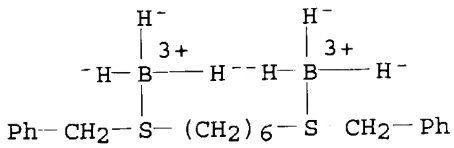


L3 25 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Boron, trihydro[1,1,1,2,2,3,3,4,4,5,5,6,6-tridecafluoro-8-(methylthio-κS)octane]-, (T-4)- (9CI)
MF C9 H10 B F13 S
CI CCS

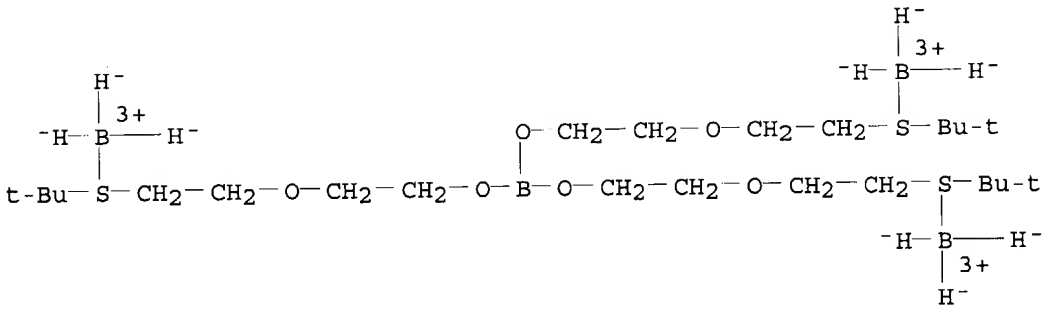


L3 25 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Boron, [μ-[1,1'-[1,6-hexanediylbis(thiomethylene)]bis[benzene]-S:S']]hexahydrodi- (9CI)

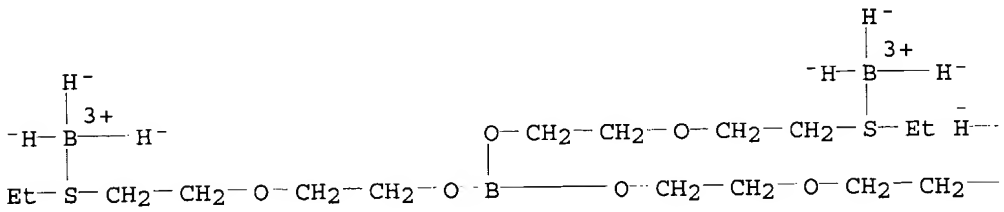
MF C20 H32 B2 S2
CI CCS

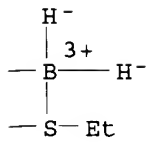


L3 25 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Boron, nonahydro[μ3-[tris[2-[2-[(1,1-dimethylethyl)thio-κS]ethoxy]ethyl] orthoborate]]tri- (9CI)
MF C24 H60 B4 O6 S3
CI CCS



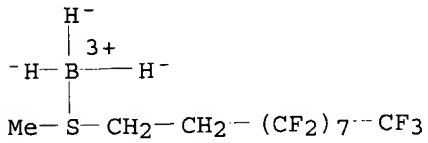
L3 25 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Boron, nonahydro[μ3-[tris[2-[2-(ethylthio-κS)ethoxy]ethyl] orthoborate]]tri- (9CI)
MF C18 H48 B4 O6 S3
CI CCS



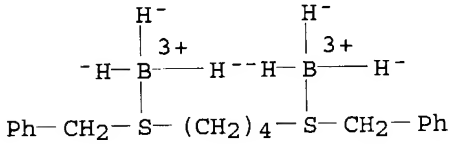


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

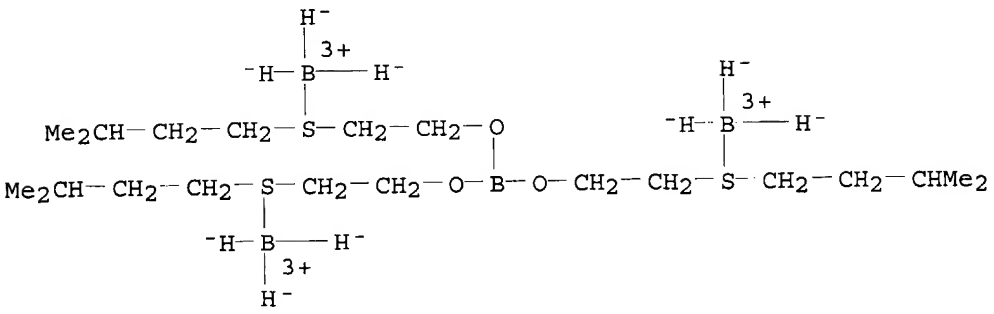
L3 25 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Boron, [1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio-κS)decane]trihydro-, (T-4)- (9CI)
MF C11 H10 B F17 S
CI CCS



L3 25 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Boron, [μ-[1,1'-[1,4-butanediylbis(thiomethylene)]bis[benzene]-S:S']]hexahydro- (9CI)
MF C18 H28 B2 S2
CI CCS

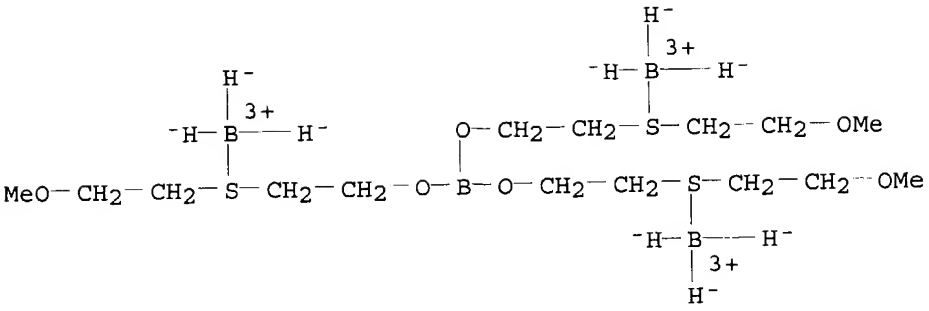


L3 25 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Boron, nonahydro[μ3-[tris[2-[(3-methylbutyl)thio-κS]ethyl]orthoborate]]tri- (9CI)
MF C21 H54 B4 O3 S3
CI CCS

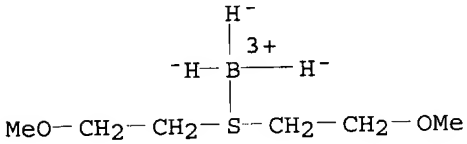


L3 25 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Boron, nonahydro[μ3-[tris[2-[(2-methoxyethyl)thio-κS]ethyl]orthoborate]]tri- (9CI)
MF C15 H42 B4 O6 S3

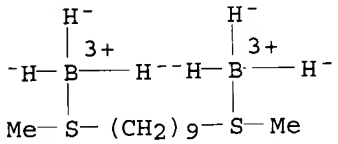
CI CCS



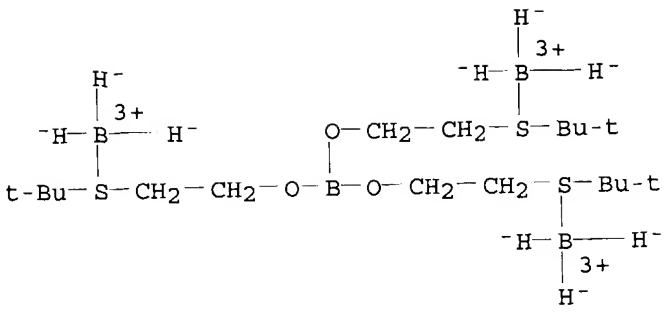
L3 25 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Boron, trihydro[1,1'-(thio-κS)bis[2-methoxyethane]]-, (T-4)- (9CI)
MF C6 H17 B O2 S
CI CCS



L3 25 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Boron, [μ-[1,9-bis(methylthio)nonane-S:S']]hexahydrodi- (9CI)
MF C11 H30 B2 S2
CI CCS

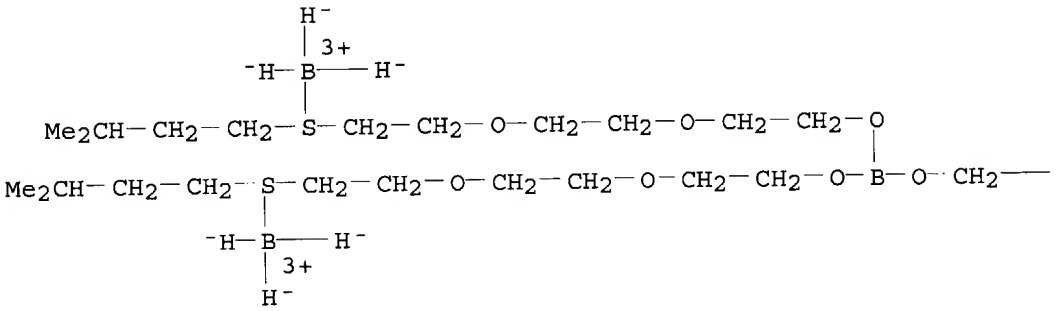


L3 25 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Boron, nonahydro[μ3-[tris[2-[(1,1-dimethylethyl)thio-κS]ethyl]
orthoborate]]tri- (9CI)
MF C18 H48 B4 O3 S3
CI CCS

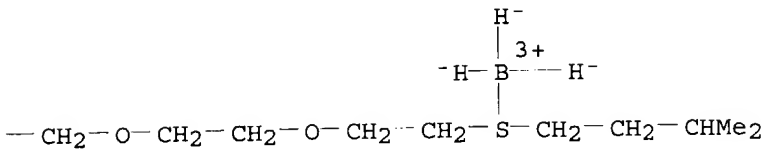


L3 25 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Boron, nonahydro[μ3-[tris[2-[2-[2-[(3-methylbutyl)thio-κS]ethoxy]ethoxy]ethyl] orthoborate]]tri- (9CI)
MF C33 H78 B4 O9 S3
CI CCS

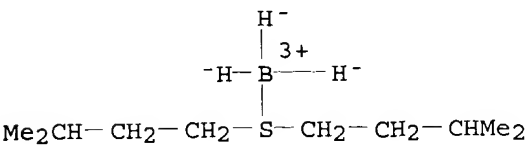
PAGE 1-A



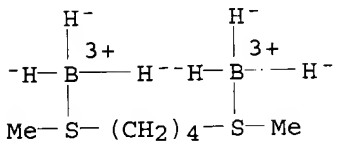
PAGE 1-B



L3 25 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Boron, trihydro[1,1'-thiobis[3-methylbutane]]-, (T-4)- (9CI)
MF C10 H25 B S
CI CCS

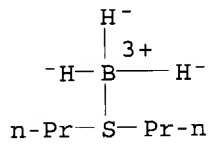


L3 25 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Boron, [μ-[1,4-bis(methylthio)butane-S:S']]hexahydrodi- (9CI)
MF C6 H20 B2 S2
CI CCS

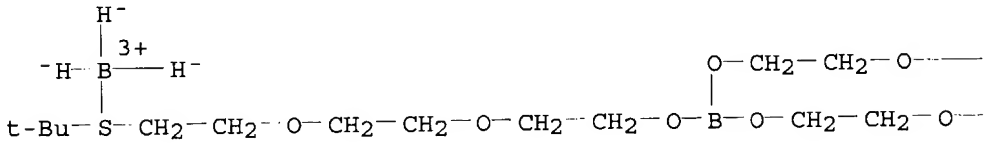


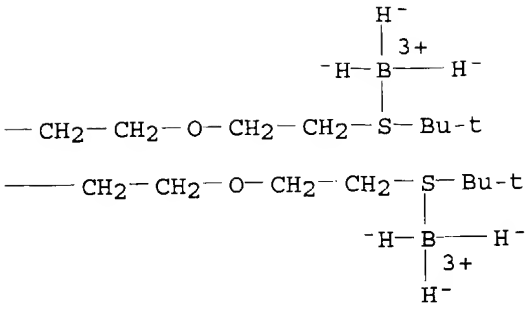
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L3 25 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Boron, trihydro[1,1'-thiobis[propane]]-, (T-4)- (9CI)
MF C6 H17 B S
CI CCS

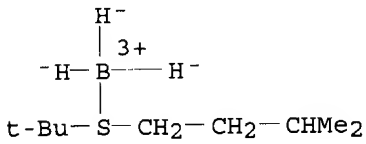


L3 25 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Boron, nonahydro[μ3-[tris[2-[2-[2-[(1,1-dimethylethyl)thio-
κS]ethoxy]ethoxy]ethyl] orthoborate]]tri- (9CI)
MF C30 H72 B4 O9 S3
CI CCS

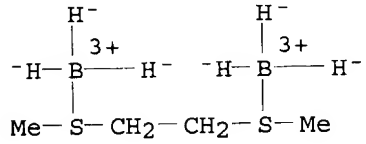




L3 25 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Boron, [1-[(1,1-dimethylethyl)thio]-3-methylbutane]trihydro-, (T-4)- (9CI)
MF C9 H23 B S
CI CCS



L3 25 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Boron, [μ-[1,2-bis(methylthio)ethane-S:S']]hexahydro- (9CI)
MF C4 H16 B2 S2
CI CCS

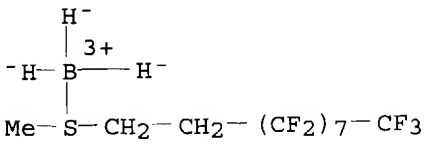


ALL ANSWERS HAVE BEEN SCANNED

=> s l3 and 1/b
263766 1/B
L4 9 L3 AND 1/B

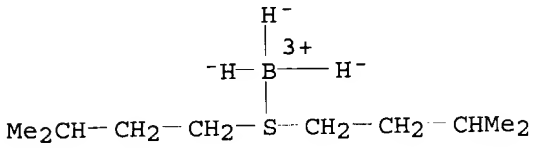
=> d scan

L4 9 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Boron, [1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio-κS)decane]trihydro-, (T-4)- (9CI)
MF **C11 H10 B F17 S**
CI CCS

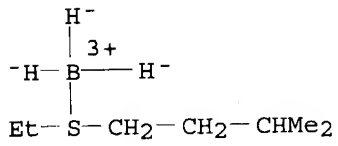


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

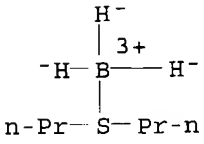
L4 9 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Boron, trihydro[1,1'-thiobis[3-methylbutane]]-, (T-4)- (9CI)
MF **C10 H25 B S**
CI CCS



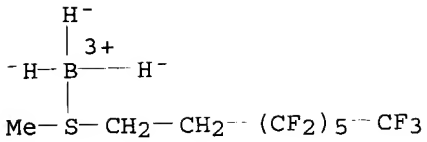
L4 9 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Boron, [1-(ethylthio)-3-methylbutane]trihydro-, (T-4)- (9CI)
MF **C7 H19 B S**
CI CCS



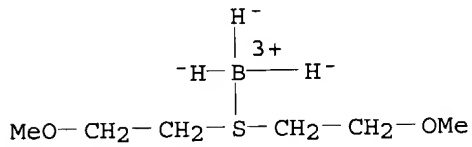
L4 9 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Boron, trihydro[1,1'-thiobis[propane]]-, (T-4)- (9CI)
MF **C6 H17 B S**
CI CCS



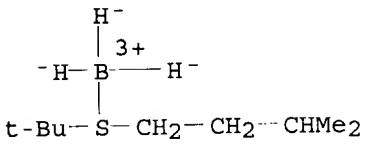
L4 9 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Boron, trihydro[1,1,1,2,2,3,3,4,4,5,5,6,6-tridecafluoro-8-(methylthio-κS)octane]-, (T-4)- (9CI)
MF **C9 H10 B F13 S**
CI CCS



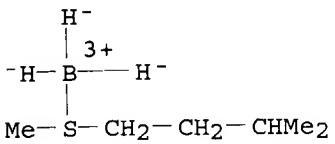
L4 9 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Boron, trihydro[1,1'-(thio-κS)bis[2-methoxyethane]]-, (T-4)- (9CI)
MF **C6 H17 B O2 S**
CI CCS



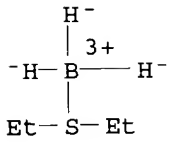
L4 9 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Boron, [1-[(1,1-dimethylethyl)thio]-3-methylbutane]trihydro-, (T-4)- (9CI)
MF **C9 H23 B S**
CI CCS



L4 9 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Boron, trihydro[3-methyl-1-(methylthio)butane]-, (T-4)- (9CI)
MF **C6 H17 B S**
CI CCS



L4 9 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Boron, trihydro[1,1'-thiobis[ethane]]-, (T-4)- (9CI)
MF **C4 H13 B S**
CI CCS



ALL ANSWERS HAVE BEEN SCANNED

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	160.27	160.90

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FILE LAST UPDATED: 11 May 2004 (20040511/ED)

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=> s l4
L5 7 L4

=> d ibib abs hitstr 1-7

L5 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2004:101171 CAPLUS
DOCUMENT NUMBER: 140:163242
TITLE: Preparation of recyclable fluorous borane-sulfides and their use in the large-scale hydroboration of alkenes or alkynes and reduction of organic functional groups
INVENTOR(S): Crich, David C.; Neelamkavil, Santhosh
PATENT ASSIGNEE(S): The Board of Trustees of the University of Illinois, USA
SOURCE: PCT Int. Appl., 40 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004011472	A2	20040205	WO 2003-US22984	20030724

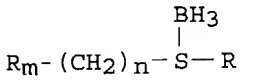
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

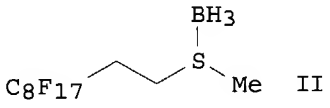
PRIORITY APPLN. INFO.: US 2002-398414P P 20020725

OTHER SOURCE(S): MARPAT 140:163242

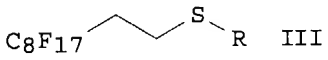
GI



I



II



III

AB The invention refers to recyclable fluorous borane-sulfide compds. of formula I [wherein: Rm = fluorinated alkyl; R = alkyl, -(CH2)2-Rm; n = 1-3] useful for large-scale hydroboration of alkenes or alkynes, or reduction of organic functional groups. To overcame disadvantages (such as liberation of stoichiometric amts. of extremely volatile, foul-smelling, and environmentally unacceptable Me2S) associated with prior synthetic methods using a borane-sulfide complex, the invention proposes the use of similar fluorous sulfides as readily prepared, odorless, nonflammable sulfides for complexation and stabilization of borane. An important addnl. feature of the invention is a recovery of the fluorous sulfides with high yields, followed by boronation to regenerate I. Fluorous borane-sulfide II was prepared via reaction of potassium thioacetate with C8F17(CH2)2I, substitution of the acetyl-group of obtained compound III (R = Ac) by Me (using NaOMe and MeI), and subsequent boronation of IV (III, R = Me). For instance, 2-MeC6H4(CH2)2NH2 was prepared via reduction of 2-MeC6H4CH2CN by a 1:1 mixture of compds. II and IV with a yield of 81% (88% of IV was recovered).

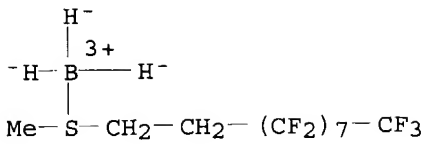
IT **478308-95-1P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

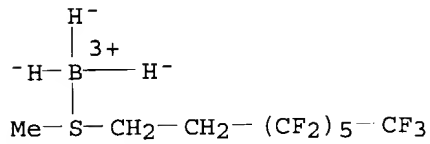
(preparation of recyclable fluorous borane-sulfides and their use in large-scale hydroboration of alkenes or alkynes and reduction of organic functional groups)

RN 478308-95-1 CAPLUS

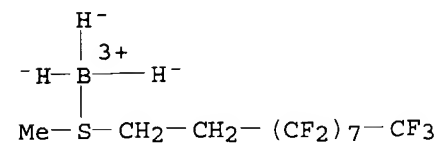
CN Boron, [1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio-κS)decane]trihydro-, (T-4)- (9CI) (CA INDEX NAME)



IT **655226-78-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of recyclable fluorous borane-sulfides and their use in large-scale hydroboration of alkenes or alkynes and reduction of organic functional groups)
RN 655226-78-1 CAPLUS
CN Boron, trihydro[1,1,1,2,2,3,3,4,4,5,5,6,6-tridecafluoro-8-(methylthio-κS)octane]-, (T-4)- (9CI) (CA INDEX NAME)



L5 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:768754 CAPLUS
DOCUMENT NUMBER: 138:24318
TITLE: Fluorous Dimethyl Sulfide: A Convenient, Odorless, Recyclable Borane Carrier
AUTHOR(S): Crich, David; Neelamkavil, Santhosh
CORPORATE SOURCE: Department of Chemistry, University of Illinois, Chicago, IL, 60607-7061, USA
SOURCE: Organic Letters (2002), 4(23), 4175-4177
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:24318
AB Borane gas and 2-(perfluorooctyl)ethyl Me sulfide form a solid comprised of an approx. 1:1 mixture (fluorous BMS) of sulfide and the corresponding sulfide-borane. Fluorous BMS permits hydroboration of alkenes in a dichloromethane/perfluorinated hydrocarbon mixture with subsequent recycling of the fluorous sulfide by fluorous extraction The use of fluorous BMS in the asym. reduction of ketones catalyzed by a chiral oxazaborolidine catalyst, and in the reduction of other functional groups, is also reported.
IT **478308-95-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(fluorous di-Me sulfide as recyclable borane carrier in hydroboration and reduction reactions)
RN 478308-95-1 CAPLUS
CN Boron, [1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio-κS)decane]trihydro-, (T-4)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:195218 CAPLUS
DOCUMENT NUMBER: 134:207964
TITLE: Economical and convenient procedures for the synthesis of catecholborane
INVENTOR(S): Brown, Herbert C.
PATENT ASSIGNEE(S): Sigma-Aldrich Co., USA
SOURCE: U.S., 6 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

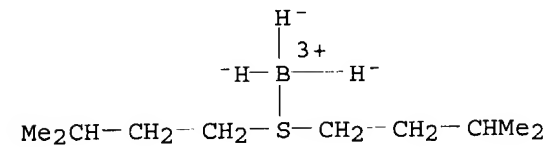
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6204405	B1	20010320	US 1999-469274	19991222

PRIORITY APPLN. INFO.: US 1999-469274 19991222
OTHER SOURCE(S): CASREACT 134:207964

AB New, economical and convenient procedures for the preparation of catecholborane in high CP form using tri-O-phenylene bis borate, readily prepared from reaction of catechol with boric acid, and diborane or borane-Lewis base complexes is described. Thus, reaction of catechol with boric acid in PhMe gave tri-O-phenylene bis borate which on treatment with diborane gas gave catecholborane with 98% purity.

IT **183118-10-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with tri-O-phenylene bis borate)

RN 183118-10-7 CAPLUS
CN Boron, trihydro[1,1'-thiobis[3-methylbutane]]-, (T-4)- (9CI) (CA INDEX NAME)



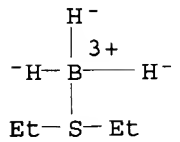
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:609227 CAPLUS
DOCUMENT NUMBER: 133:335260
TITLE: Molecular Addition Compounds. 17. Borane and Chloroborane Adducts with Organic Sulfides for Hydroboration
AUTHOR(S): Zaidlewicz, Marek; Kanth, Josyula V. B.; Brown, Herbert C.
CORPORATE SOURCE: H. C. Brown Center for Borane Research, Purdue University, West Lafayette, IN, 47907, USA
SOURCE: Journal of Organic Chemistry (2000), 65(20), 6697-6702
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:335260

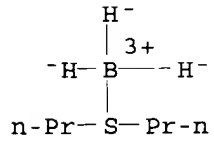
AB The following sulfides were examined as borane carriers in comparison with di-Me sulfide and 1,4-oxathiane: tert-Bu Me sulfide, isoamyl Me sulfide, Et isoamyl sulfide, tert-Bu isoamyl sulfide, diisoamyl sulfide, tetrahydrothiophene, tetrahydro-thiopyran, thioanisole, 3-ethylthiotetrahydrofuran, bis(3-tetrahydrofuryl) sulfide, and bis(2-methoxyethyl) sulfide. Their complexing ability toward borane increases in the following order: thioanisole < ether-sulfides < dialkyl sulfides < di-Me sulfide. Borane adducts of the sulfides are liqs. >0°. The thioanisole adduct loses diborane at room temperature The reactivity of the adducts toward 1-octene increases in the reversed order of the complexing ability of the sulfides. Diisoamyl sulfide has a mild, ethereal, agreeable aroma, its synthesis is economical and the borane adduct, 4.2M in BH3, is stable over prolonged periods at room temperature The sulfide can be recovered from hydroboration-oxidation products by distillation Consequently, diisoamyl sulfide is a new promising borane carrier. Bis(2-methoxyethyl) sulfide, easily synthesized from the low cost thiodiethanol, is three times more soluble in H2O than 1,4-oxathiane. Its borane adduct is 6.0M in BH3 and can substitute for more expensive borane-1,4-oxathiane in hydroboration reactions. Applications of these new borane adducts in the synthesis of mono- and dichloroborane adducts was also studied. The equilibrium ratios observed for the new chloroborane adducts were similar to that observed for di-Me sulfide adducts. However, the hydroboration of 1-octene with these new chloroborane adducts are much faster than the corresponding adducts of di-Me sulfide, which are currently used extensively.

IT **55606-71-8 151183-12-9 183118-06-1 183118-08-3 183118-09-4 183118-10-7 183118-13-0**
RL: FMU (Formation, unclassified); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
(formation and hydroboration of alkenes by)

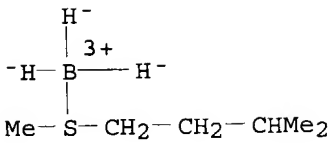
RN 55606-71-8 CAPLUS
CN Boron, trihydro[1,1'-thiobis[ethane]]-, (T-4)- (9CI) (CA INDEX NAME)



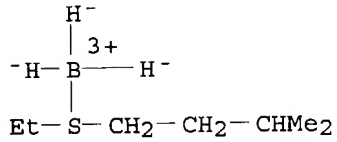
RN 151183-12-9 CAPLUS
CN Boron, trihydro[1,1'-thiobis[propane]]-, (T-4)- (9CI) (CA INDEX NAME)



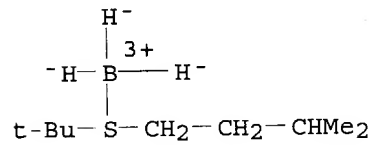
RN 183118-06-1 CAPLUS
CN Boron, trihydro[3-methyl-1-(methylthio)butane]-, (T-4)- (9CI) (CA INDEX NAME)



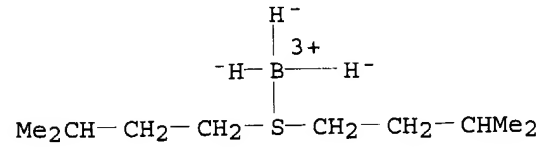
RN 183118-08-3 CAPLUS
CN Boron, [1-(ethylthio)-3-methylbutane]trihydro-, (T-4)- (9CI) (CA INDEX NAME)



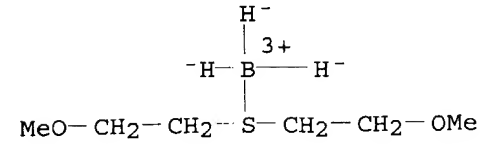
RN 183118-09-4 CAPLUS
CN Boron, [1-[(1,1-dimethylethyl)thio]-3-methylbutane]trihydro-, (T-4)- (9CI) (CA INDEX NAME)



RN 183118-10-7 CAPLUS
CN Boron, trihydro[1,1'-thiobis[3-methylbutane]]-, (T-4)- (9CI) (CA INDEX NAME)



RN 183118-13-0 CAPLUS
CN Boron, trihydro[1,1'-(thio-κS)bis[2-methoxyethane]]-, (T-4)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1996:657071 CAPLUS
DOCUMENT NUMBER: 125:301225
TITLE: Borane-sulfide hydroboration agents
INVENTOR(S): Brown, Herbert C.
PATENT ASSIGNEE(S): Aldrich Chemical Company, Inc., USA
SOURCE: U.S., 6 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

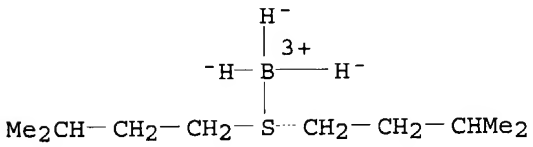
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5567849	A	19961022	US 1995-437582	19950509

PRIORITY APPLN. INFO.: US 1995-437582 19950509
OTHER SOURCE(S): MARPAT 125:301225

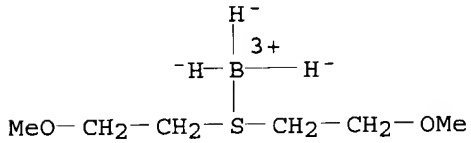
AB A borane-sulfide represented by the formula BH3.SR1R2 wherein R1 and R2 each are straight or branched chain alkyl or alkoxy with at least one R being a branched chain when both R1 and R2 are alkyl is described. The compds. are hydroboration agents.

IT **183118-10-7P 183118-13-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydroboration with)

RN 183118-10-7 CAPLUS
CN Boron, trihydro[1,1'-thiobis[3-methylbutane]]-, (T-4)- (9CI) (CA INDEX NAME)

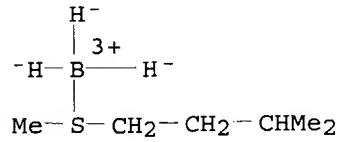


RN 183118-13-0 CAPLUS
CN Boron, trihydro[1,1'-(thio-κS)bis[2-methoxyethane]]-, (T-4)- (9CI) (CA INDEX NAME)

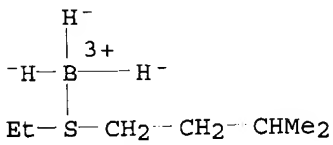


IT **183118-06-1P 183118-08-3P 183118-09-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

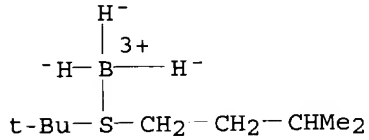
RN 183118-06-1 CAPLUS
CN Boron, trihydro[3-methyl-1-(methylthio)butane]-, (T-4)- (9CI) (CA INDEX NAME)



RN 183118-08-3 CAPLUS
CN Boron, [1-(ethylthio)-3-methylbutane]trihydro-, (T-4)- (9CI) (CA INDEX NAME)



RN 183118-09-4 CAPLUS
CN Boron, [1-[(1,1-dimethylethyl)thio]-3-methylbutane]trihydro-, (T-4)- (9CI) (CA INDEX NAME)



L5 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1991:414091 CAPLUS
DOCUMENT NUMBER: 115:14091
TITLE: Borane-organosilicon preceramic polymers, their manufacture, and ceramics formed from these polymers
INVENTOR(S): Seyferth, Dietmar; Plenio, Herbert
PATENT ASSIGNEE(S): Massachusetts Institute of Technology, USA
SOURCE: Eur. Pat. Appl., 28 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

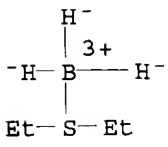
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 424082	A2	19910424	EP 1990-311309	19901016
EP 424082	A3	19910710		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
US 5171736	A	19921215	US 1989-421586	19891016
CA 2027669	AA	19910417	CA 1990-2027669	19901015
JP 03221531	A2	19910930	JP 1990-277602	19901016

PRIORITY APPLN. INFO.: US 1989-421586 19891016

AB The polymers are the reaction products of multiple Si-H and Si-N functional group-containing organosilicon oligomers or polymers and a borane, with the molar ratio of organosilicon polymer repeating units:borane being ≤15:1. The ceramics are formed by pyrolyzing the preceramic polymers. The preceramic polymers are soluble in organic solvents and/or fusible, and give high Si nitride-B nitride yields.

IT **55606-71-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with silazanes, for preceramic polymers)

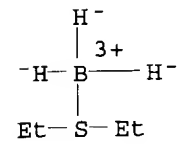
RN 55606-71-8 CAPLUS
CN Boron, trihydro[1,1'-thiobis[ethane]]-, (T-4)- (9CI) (CA INDEX NAME)



L5 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1975:541236 CAPLUS
DOCUMENT NUMBER: 83:141236
TITLE: Reactions of pentaborane(11) with ethers
AUTHOR(S): Kodama, Goji; Saturnino, Dennis J.
CORPORATE SOURCE: Dep. Chem., Univ. Utah, Salt Lake City, UT, USA
SOURCE: Inorganic Chemistry (1975), 14(9), 2243-9
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Reactions of pentaborane(11) with ethers were studied at low temps. by means of 11B NMR spectroscopy. The reactions of B5H11 with dimethyl and diethyl thioethers gave the sym. cleavage products R2S.BH3 and R2S.B4H8. Species that are produced in the reaction system of B5H11 and oxoethers are very dependent upon the base strength of the ether. Strongly basic THF can effect the unsym. cleavage of B5H11 to produce H2B(THF)2+B4H9-. Evidence for the formation of this cleavage product is based on NMR spectral evidence and on the observed reaction products produced in the reaction of HCl with the B5H11-THF system. A 2nd species is observable in the THF-B5H11 system which is more predominant at higher temps. This species is the simple adduct B5H11.THF. Moderately basic ethers like Me2O and Et2O produce only 1 observable species which is considered to be B5H11.OR2. Weakly basic iso-Pr2O does not react with B5H11. No direct evidence for the sym. cleavage of B5H11 by oxoethers was observed The similarities and differences between these reactions and analogous B4H10 reactions are discussed.

IT **55606-71-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 55606-71-8 CAPLUS
CN Boron, trihydro[1,1'-thiobis[ethane]]-, (T-4)- (9CI) (CA INDEX NAME)



=> FIL CASREACT

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	35.92	196.82

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-4.85	-4.85

FILE 'CASREACT' ENTERED AT 15:22:51 ON 12 MAY 2004

FILE CONTENT:1840 - 9 May 2004 VOL 140 ISS 19

Some records from 1974 to 1991 are derived from the ZIC/VINITI data file and provided by InfoChem and some records are produced using some INPI data from the period prior to 1986.

This file contains CAS Registry Numbers for easy and accurate substance identification.

Crossover limits have been increased. See HELP RNCROSSOVER for details.

Structure search limits have been raised. See HELP SLIMIT for the new, higher limits.

=> D ACC 138:24318 ALL

ANSWER 1 CASREACT COPYRIGHT 2004 ACS on STN
AN 138:24318 CASREACT
TI Fluorous Dimethyl Sulfide: A Convenient, Odorless, Recyclable Borane Carrier
AU Crich, David; Neelamkavil, Santhosh
CS Department of Chemistry, University of Illinois, Chicago, IL, 60607-7061, USA
SO Organic Letters (2002), 4(23), 4175-4177
CODEN: ORLEF7; ISSN: 1523-7060
PB American Chemical Society
DT Journal
LA English
CC 21-2 (General Organic Chemistry)
AB Borane gas and 2-(perfluorooctyl)ethyl Me sulfide form a solid comprised of an approx. 1:1 mixture (fluorous BMS) of sulfide and the corresponding sulfide-borane. Fluorous BMS permits hydroboration of alkenes in a dichloromethane/perfluorinated hydrocarbon mixture with subsequent recycling of the fluorous sulfide by fluorous extraction The use of fluorous BMS in the asym. reduction of ketones catalyzed by a chiral oxazaborolidine catalyst, and in the reduction of other functional groups, is also reported.
ST fluorous borane sulfide prepn hydroboration asym redn; olefin hydroboration fluorous borane sulfide; ketone asym redn oxazaborolidine fluorous borane sulfide; ester redn fluorous borane sulfide; nitrile redn fluorous borane sulfide; amide redn fluorous borane sulfide
IT Hydroboration
Reduction
(fluorous di-Me sulfide as recyclable borane carrier in hydroboration and reduction reactions)
IT Alkenes, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(fluorous di-Me sulfide as recyclable borane carrier in hydroboration and reduction reactions)
IT Alcohols, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(fluorous di-Me sulfide as recyclable borane carrier in hydroboration and reduction reactions)
IT Reduction
(stereoselective; of acetophenone with fluorous di-Me sulfide as recyclable borane carrier)

IT 110205-59-9
RL: CAT (Catalyst use); USES (Uses)
(fluorous di-Me sulfide as recyclable borane carrier in hydroboration and reduction reactions)
IT 98-86-2, Acetophenone, reactions 127-91-3, β-Pinene 591-49-1, 1-Methylcyclohexene 2043-53-0 10387-40-3, Potassium thioacetate 13389-42-9, trans-2-Octene 17416-73-8 22049-87-2 22364-68-7 157989-22-5 219937-71-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(fluorous di-Me sulfide as recyclable borane carrier in hydroboration and reduction reactions)
IT 19287-45-7P, Diborane 125640-21-3P 478296-48-9P 478308-95-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(fluorous di-Me sulfide as recyclable borane carrier in hydroboration and reduction reactions)
IT 123-96-6P, 2-Octanol 589-98-0P, 3-Octanol 1517-69-7P, (R)-1-Phenylethanol 7443-52-9P, trans-2-Methylcyclohexanol 15358-92-6P, cis-Myrtanol 55755-16-3P 145510-21-0P 448957-53-7P 478296-49-0P 478296-50-3P 478296-51-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(fluorous di-Me sulfide as recyclable borane carrier in hydroboration and reduction reactions)
IT 16940-66-2, Sodium borohydride
RL: RCT (Reactant); RACT (Reactant or reagent)
(prereactant with boron trifluoride etherate; fluorous di-Me sulfide as recyclable borane carrier in hydroboration and reduction reactions)
IT 109-63-7, Boron trifluoride etherate
RL: RCT (Reactant); RACT (Reactant or reagent)
(prereactant with sodium borohydride; fluorous di-Me sulfide as recyclable borane carrier in hydroboration and reduction reactions)
RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE

(1) Braun, L; J Org Chem 1971, V36, P2388
(2) Brown, H; J Am Chem Soc 1961, V83, P2544 CAPLUS
(3) Brown, H; J Am Chem Soc 1970, V92, P1637 CAPLUS
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(5) Brown, H; J Org Chem 1992, V57, P4970 CAPLUS
(6) Brown, H; J Org Chem 2001, V66, P4795 CAPLUS
(7) Brown, H; Organic Synthesis via Boranes 1975
(8) Bruncko, M; J Org Chem 1994, V59, P5543 CAPLUS
(9) Corey, E; Angew Chem, Int Ed 1998, V37, P1987
(10) Corrie, J; J Chem Soc, Perkin Trans 1 1996, P1583 CAPLUS
(11) Crich, D; J Am Chem Soc 2001, V123, P7449 CAPLUS
(12) Crich, D; Org Lett 1999, V1, P269 CAPLUS
(13) Crich, D; Org Lett 2000, V2, P4029 CAPLUS
(14) Crich, D; Org Lett 2000, V2, P989 CAPLUS
(15) Crich, D; Org Lett 2002, V4, P2573 CAPLUS
(16) Crich, D; Tetrahedron 1999, V55, P14261 CAPLUS
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(21) Follet, M; Chem Ind 1986, P123 CAPLUS
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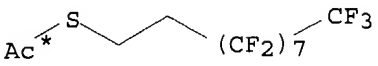
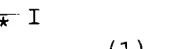
(27) Zaidlewicz, M; EROS 1995, V1, P638
(28) Zweifel, G; J Am Chem Soc 1964, V86, P393 CAPLUS
(29) Zweifel, G; Org React 1963, V13, P1 CAPLUS

RX(1) OF 15 ...A + B ===> C...



A



B

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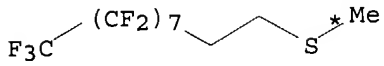


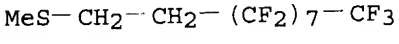
C
YIELD 94%

RX(1) RCT A 125640-21-3

STAGE(1)
RGT D 124-41-4 NaOMe
SOL 67-56-1 MeOH

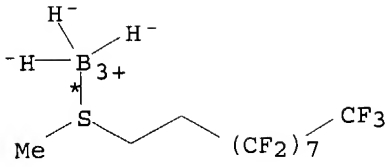
STAGE(2)
RCT B 74-88-4
PRO C 478296-48-9

RX(2) OF 15 ...C ===> F



C

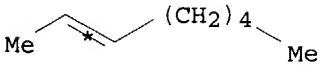
(2) →



F

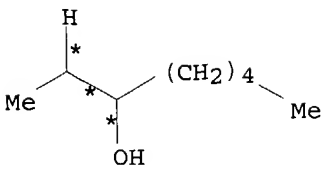
RX(2) RCT C 478296-48-9
RGT G 19287-45-7 B2H6
PRO F 478308-95-1
NTE reagent generated in situ

RX(3) OF 15 2 H ===> I + J

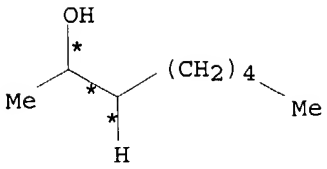


2 H

(3) →



I
YIELD 90%(45)



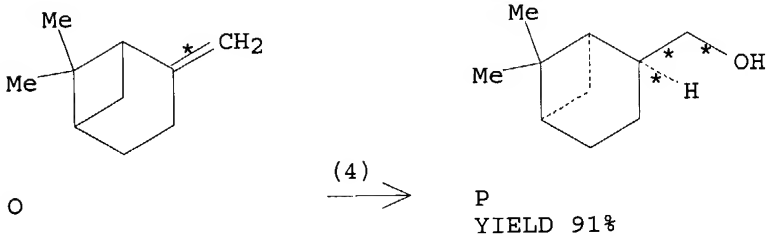
J
YIELD 90%(55)

RX(3) RCT H 13389-42-9

STAGE(1)
RGT F 478308-95-1 Boron, [1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio-κS)decane]trihydro-, (T-4)-, C 478296-48-9 Decane, 1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio)-
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT K 1310-73-2 NaOH, L 7722-84-1 H2O2
SOL 7732-18-5 Water
PRO I 589-98-0, J 123-96-6
NTE stereoselective

RX(4) OF 15 O ===> P



O

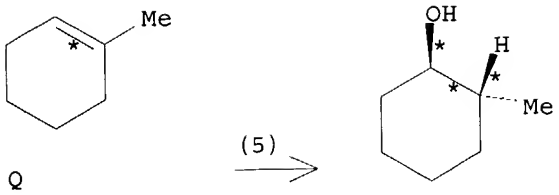
P
YIELD 91%

RX(4) RCT O 127-91-3

STAGE(1)
RGT F 478308-95-1 Boron, [1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio-κS)decane]trihydro-, (T-4)-, C 478296-48-9 Decane, 1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio)-
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT K 1310-73-2 NaOH, L 7722-84-1 H2O2
SOL 7732-18-5 Water
PRO P 15358-92-6
NTE stereoselective

RX(5) OF 15 Q ===> R



Q

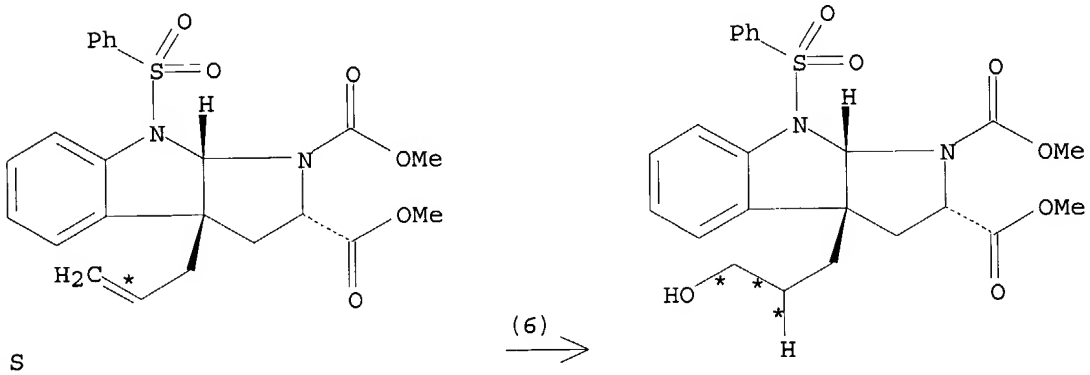
R
YIELD 91%

RX(5) RCT Q 591-49-1

STAGE(1)
RGT F 478308-95-1 Boron, [1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio-κS)decane]trihydro-, (T-4)-, C 478296-48-9 Decane, 1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio)-
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT K 1310-73-2 NaOH, L 7722-84-1 H2O2
SOL 7732-18-5 Water
PRO R 7443-52-9
NTE stereoselective

RX(6) OF 15 S ===> T



S

T
YIELD 81%

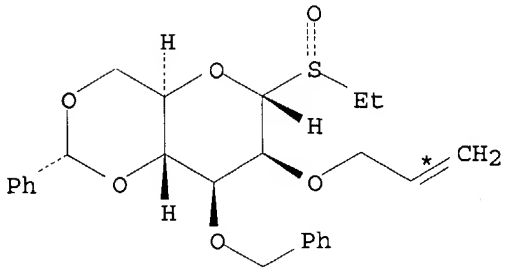
RX(6) RCT S 157989-22-5

STAGE(1)
RGT F 478308-95-1 Boron, [1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio-κS)decane]trihydro-, (T-4)-, C 478296-48-9 Decane, 1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio)-
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT K 1310-73-2 NaOH, L 7722-84-1 H2O2
SOL 7732-18-5 Water

PRO T 478296-49-0
NTE stereoselective

RX(7) OF 15 2 U ===> V + W



2 U

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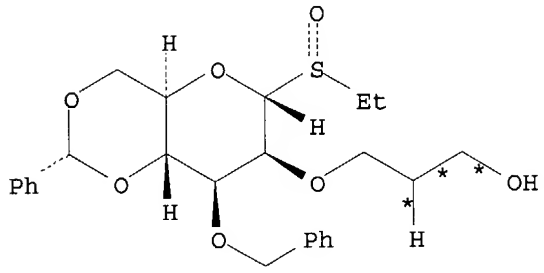
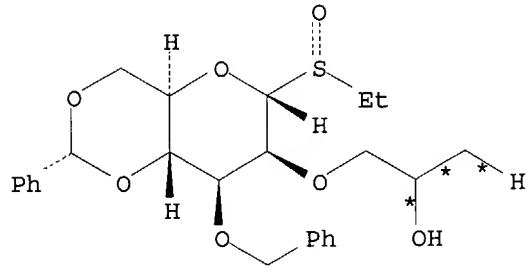


V
YIELD 78%(75)



W
YIELD 78%(25)

RX(7) RCT U 219937-71-0

STAGE(1)
RGT F 478308-95-1 Boron, [1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio-κS)decane]trihydro-, (T-4)-, C 478296-48-9 Decane, 1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio)-

SOL 75-09-2 CH2Cl2

STAGE(2)
RGT K 1310-73-2 NaOH, L 7722-84-1 H2O2
SOL 7732-18-5 Water
PRO V 478296-50-3, W 478296-51-4
NTE stereoselective

RX(8) OF 15 X ===> Y

X

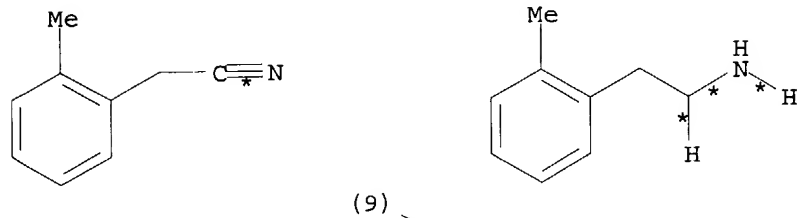
Y
YIELD 83%

RX(8) RCT X 22049-87-2

STAGE(1)
RGT F 478308-95-1 Boron, [1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio-κS)decane]trihydro-, (T-4)-, C 478296-48-9 Decane, 1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio)-
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT K 1310-73-2 NaOH, L 7722-84-1 H2O2
SOL 7732-18-5 Water
PRO Y 145510-21-0

RX(9) OF 15 Z ===> AA



Z

AA
YIELD 81%

RX(9) RCT Z 22364-68-7

STAGE(1)
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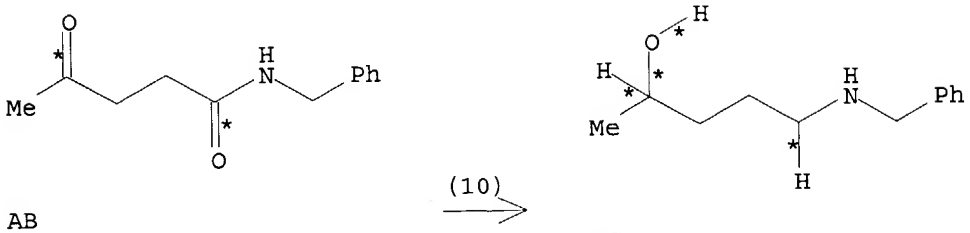
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT K 1310-73-2 NaOH, L 7722-84-1 H2O2
SOL 7732-18-5 Water
PRO AA 55755-16-3

RX(10) OF 15 AB ===> AC



AB

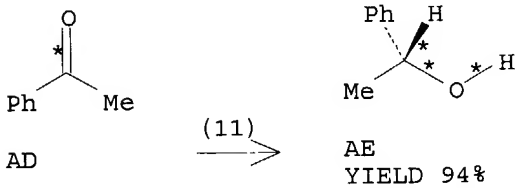
AC
YIELD 79%

RX(10) RCT AB 17416-73-8

STAGE(1)
RGT F 478308-95-1 Boron, [1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio-κS)decane]trihydro-, (T-4)-, C 478296-48-9 Decane, 1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio)-
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT K 1310-73-2 NaOH, L 7722-84-1 H2O2
SOL 7732-18-5 Water
PRO AC 448957-53-7

RX(11) OF 15 AD ===> AE

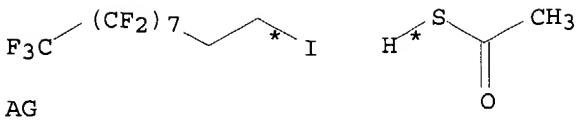


AD

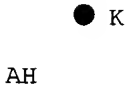
AE
YIELD 94%

RX(11) RCT AD 98-86-2
RGT F 478308-95-1 Boron, [1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio-κS)decane]trihydro-, (T-4)-
PRO AE 1517-69-7
CAT 110205-59-9 1H,3H-Pyrrolo[1,2-c][1,3,2]oxazaborole, tetrahydro-3,3-diphenyl-, (3aS)-
SOL 75-09-2 CH2Cl2
NTE stereoselective

RX(12) OF 15 AG + AH ===> A...

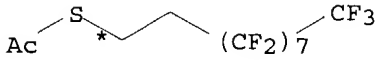


AG



AH

(12)



A
YIELD 81%

RX(12) RCT AG 2043-53-0, AH 10387-40-3
PRO A 125640-21-3
SOL 68-12-2 DMF

=> FIL CASREACT

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	16.37	213.19

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.66	-5.51

FILE 'CASREACT' ENTERED AT 15:34:05 ON 12 MAY 2004
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

FILE CONTENT:1840 - 9 May 2004 VOL 140 ISS 19

Some records from 1974 to 1991 are derived from the ZIC/VINITI data file and provided by InfoChem and some records are produced using some INPI data from the period prior to 1986.

This file contains CAS Registry Numbers for easy and accurate substance identification.

Crossover limits have been increased. See HELP RNCROSSOVER for details.

Structure search limits have been raised. See HELP SLIMIT for the new, higher limits.

=> D ACC 138:24318 ALL

ANSWER 1 CASREACT COPYRIGHT 2004 ACS on STN
AN 138:24318 CASREACT
TI Fluorous Dimethyl Sulfide: A Convenient, Odorless, Recyclable Borane Carrier
AU Crich, David; Neelamkavil, Santhosh
CS Department of Chemistry, University of Illinois, Chicago, IL, 60607-7061, USA
SO Organic Letters (2002), 4(23), 4175-4177
CODEN: ORLEF7; ISSN: 1523-7060
PB American Chemical Society
DT Journal
LA English
CC 21-2 (General Organic Chemistry)
AB Borane gas and 2-(perfluorooctyl)ethyl Me sulfide form a solid comprised of an approx. 1:1 mixture (fluorous BMS) of sulfide and the corresponding sulfide-borane. Fluorous BMS permits hydroboration of alkenes in a dichloromethane/perfluorinated hydrocarbon mixture with subsequent recycling of the fluorous sulfide by fluorous extraction The use of fluorous BMS in the asym. reduction of ketones catalyzed by a chiral oxazaborolidine catalyst, and in the reduction of other functional groups, is also reported.
ST fluorous borane sulfide prepn hydroboration asym redn; olefin hydroboration fluorous borane sulfide; ketone asym redn oxazaborolidine fluorous borane sulfide; ester redn fluorous borane sulfide; nitrile redn fluorous borane sulfide; amide redn fluorous borane sulfide
IT Hydroboration
Reduction
(fluorous di-Me sulfide as recyclable borane carrier in hydroboration and reduction reactions)
IT Alkenes, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(fluorous di-Me sulfide as recyclable borane carrier in hydroboration and reduction reactions)
IT Alcohols, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(fluorous di-Me sulfide as recyclable borane carrier in hydroboration and reduction reactions)
IT Reduction
(stereoselective; of acetophenone with fluorous di-Me sulfide as recyclable borane carrier)
IT 110205-59-9
RL: CAT (Catalyst use); USES (Uses)
(fluorous di-Me sulfide as recyclable borane carrier in hydroboration and reduction reactions)
IT 98-86-2, Acetophenone, reactions 127-91-3, β-Pinene 591-49-1, 1-Methylcyclohexene 2043-53-0 10387-40-3, Potassium thioacetate 13389-42-9, trans-2-Octene 17416-73-8 22049-87-2 22364-68-7 157989-22-5 219937-71-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(fluorous di-Me sulfide as recyclable borane carrier in hydroboration and reduction reactions)
IT 19287-45-7P, Diborane 125640-21-3P 478296-48-9P 478308-95-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(fluorous di-Me sulfide as recyclable borane carrier in hydroboration and reduction reactions)
IT 123-96-6P, 2-Octanol 589-98-0P, 3-Octanol 1517-69-7P, (R)-1-Phenylethanol 7443-52-9P, trans-2-Methylcyclohexanol 15358-92-6P, cis-Myrtanol 55755-16-3P 145510-21-0P 448957-53-7P 478296-49-0P 478296-50-3P 478296-51-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(fluorous di-Me sulfide as recyclable borane carrier in hydroboration and reduction reactions)
IT 16940-66-2, Sodium borohydride

RL: RCT (Reactant); RACT (Reactant or reagent)
(prereactant with boron trifluoride etherate; fluorous di-Me sulfide as recyclable borane carrier in hydroboration and reduction reactions)

IT 109-63-7, Boron trifluoride etherate
RL: RCT (Reactant); RACT (Reactant or reagent)
(prereactant with sodium borohydride; fluorous di-Me sulfide as recyclable borane carrier in hydroboration and reduction reactions)

RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Braun, L; J Org Chem 1971, V36, P2388
(2) Brown, H; J Am Chem Soc 1961, V83, P2544 CAPLUS
(3) Brown, H; J Am Chem Soc 1970, V92, P1637 CAPLUS
(4) Brown, H; J Org Chem 1977, V42, P1392 CAPLUS
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(7) Brown, H; Organic Synthesis via Boranes 1975
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(11) Crich, D; J Am Chem Soc 2001, V123, P7449 CAPLUS
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(16) Crich, D; Tetrahedron 1999, V55, P14261 CAPLUS
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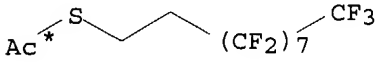
(27) Zaidlewicz, M; EROS 1995, V1, P638
(28) Zweifel, G; J Am Chem Soc 1964, V86, P393 CAPLUS
(29) Zweifel, G; Org React 1963, V13, P1 CAPLUS

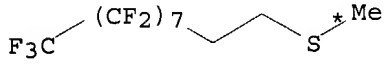
RX(1) OF 15 ...A + B ===> C...



A

B

(1)



C

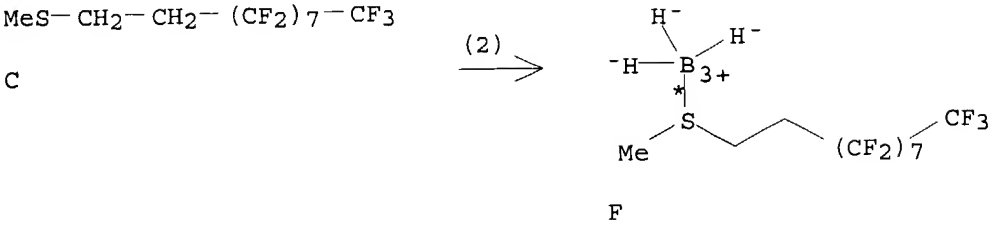
YIELD 94%

RX(1) RCT A 125640-21-3

STAGE(1)
RGT D 124-41-4 NaOMe
SOL 67-56-1 MeOH

STAGE(2)
RCT B 74-88-4
PRO C 478296-48-9

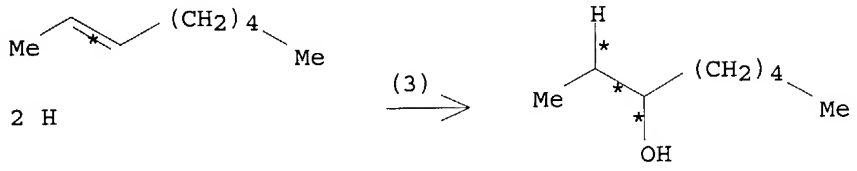
RX(2) OF 15 ...C ===> F



C F

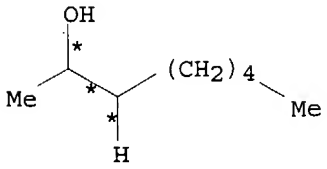
RX(2) RCT C 478296-48-9
RGT G 19287-45-7 B2H6
PRO F 478308-95-1
NTE reagent generated in situ

RX(3) OF 15 2 H ===> I + J



2 H I

YIELD 90%(45)



J

YIELD 90%(55)

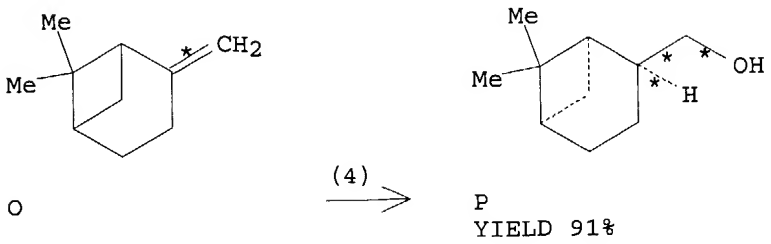
RX(3) RCT H 13389-42-9

STAGE(1)
RGT F 478308-95-1 Boron, [1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio-κS)decane]trihydro-, (T-4)-, C 478296-48-9 Decane, 1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio)-
SOL 75-09-2 CH2Cl2

STAGE(2)

RGT K 1310-73-2 NaOH, L 7722-84-1 H2O2
SOL 7732-18-5 Water
PRO I 589-98-0, J 123-96-6
NTE stereoselective

RX(4) OF 15 O ===> P



O

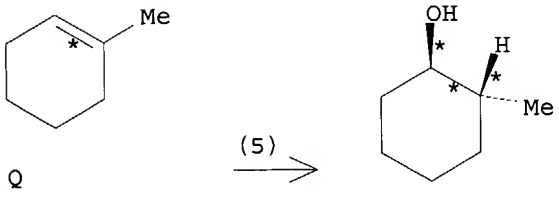
P
YIELD 91%

RX(4) RCT O 127-91-3

STAGE(1)
RGT F 478308-95-1 Boron, [1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio-κS)decane]trihydro-, (T-4)-, C 478296-48-9 Decane, 1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio)-
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT K 1310-73-2 NaOH, L 7722-84-1 H2O2
SOL 7732-18-5 Water
PRO P 15358-92-6
NTE stereoselective

RX(5) OF 15 Q ===> R



Q

R
YIELD 91%

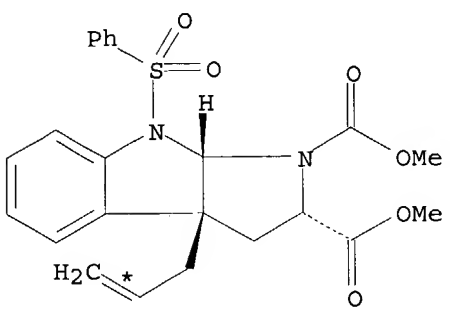
RX(5) RCT Q 591-49-1

STAGE(1)
RGT F 478308-95-1 Boron, [1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio-κS)decane]trihydro-, (T-4)-, C 478296-48-9 Decane, 1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio)-
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT K 1310-73-2 NaOH, L 7722-84-1 H2O2

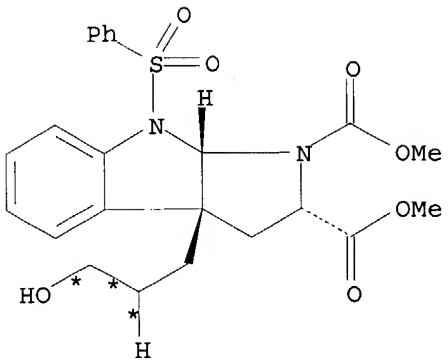
SOL 7732-18-5 Water
PRO R 7443-52-9
NTE stereoselective

RX(6) OF 15 S ===> T



S

(6)



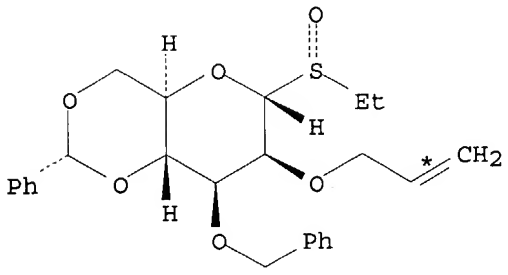
T
YIELD 81%

RX(6) RCT S 157989-22-5

STAGE(1)
RGT F 478308-95-1 Boron, [1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio-κS)decane]trihydro-, (T-4)-, C 478296-48-9 Decane, 1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio)-
SOL 75-09-2 CH2Cl2

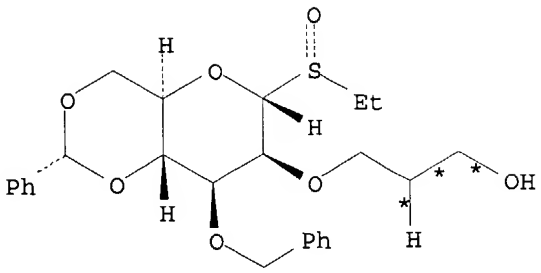
STAGE(2)
RGT K 1310-73-2 NaOH, L 7722-84-1 H2O2
SOL 7732-18-5 Water
PRO T 478296-49-0
NTE stereoselective

RX(7) OF 15 2 U ===> V + W

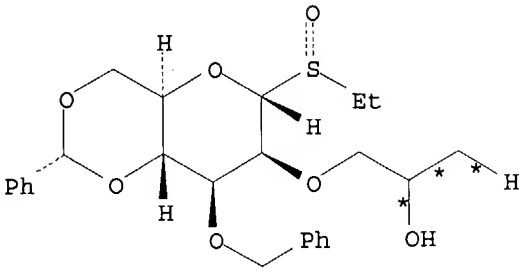


2 U

(7)



V
YIELD 78%(75)



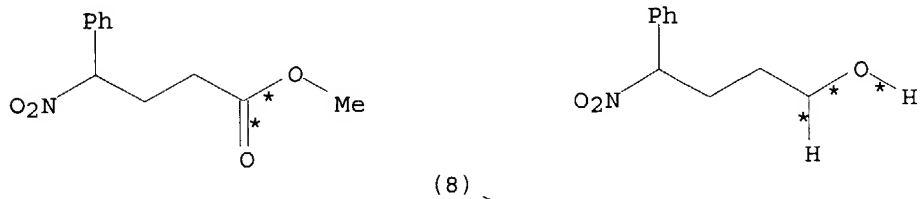
W
YIELD 78%(25)

RX(7) RCT U 219937-71-0

STAGE(1)
RGT F 478308-95-1 Boron, [1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio-κS)decane]trihydro-, (T-4)-, C 478296-48-9 Decane, 1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio)-
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT K 1310-73-2 NaOH, L 7722-84-1 H2O2
SOL 7732-18-5 Water
PRO V 478296-50-3, W 478296-51-4
NTE stereoselective

RX(8) OF 15 X ===> Y



X

(8)

Y
YIELD 83%

RX(8) RCT X 22049-87-2

STAGE(1)
RGT F 478308-95-1 Boron, [1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio-κS)decane]trihydro-, (T-4)-, C 478296-48-9 Decane, 1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio)-
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT K 1310-73-2 NaOH, L 7722-84-1 H2O2
SOL 7732-18-5 Water
PRO Y 145510-21-0

RX(9) OF 15 Z ===> AA

Z

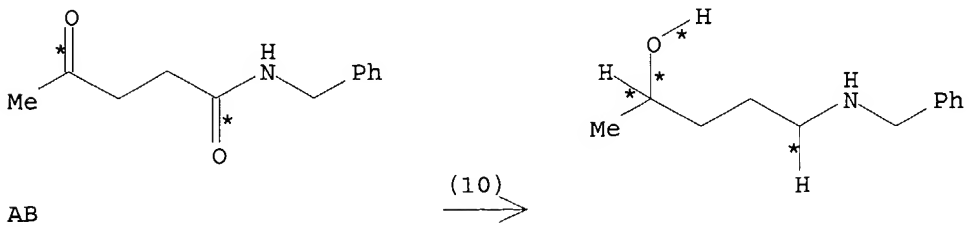
AA
YIELD 81%

RX(9) RCT Z 22364-68-7

STAGE(1)
RGT F 478308-95-1 Boron, [1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio-κS)decane]trihydro-, (T-4)-, C 478296-48-9 Decane, 1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio)-
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT K 1310-73-2 NaOH, L 7722-84-1 H2O2
SOL 7732-18-5 Water
PRO AA 55755-16-3

RX(10) OF 15 AB ===> AC



AB

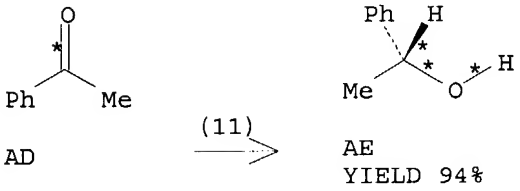
AC
YIELD 79%

RX(10) RCT AB 17416-73-8

STAGE(1)
RGT F 478308-95-1 Boron, [1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio-κS)decane]trihydro-, (T-4)-, C 478296-48-9 Decane, 1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio)-
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT K 1310-73-2 NaOH, L 7722-84-1 H2O2
SOL 7732-18-5 Water
PRO AC 448957-53-7

RX(11) OF 15 AD ===> AE

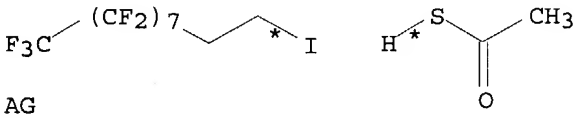


AD

AE
YIELD 94%

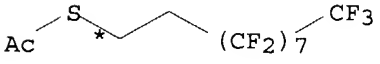
RX(11) RCT AD 98-86-2
RGT F 478308-95-1 Boron, [1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-(methylthio-κS)decane]trihydro-, (T-4)-
PRO AE 1517-69-7
CAT 110205-59-9 1H,3H-Pyrrolo[1,2-c][1,3,2]oxazaborole, tetrahydro-3,3-diphenyl-, (3aS)-
SOL 75-09-2 CH2Cl2
NTE stereoselective

RX(12) OF 15 AG + AH ===> A...



AG

AH



A
YIELD 81%

RX(12) RCT AG 2043-53-0, AH 10387-40-3
PRO A 125640-21-3

SOL 68-12-2 DMF

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=> file beilstein
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                      10.49     223.68

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                         ENTRY    SESSION
CA SUBSCRIBER PRICE                                      -0.66      -6.17

FILE 'BEILSTEIN' ENTERED AT 15:36:56 ON 12 MAY 2004
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FILE RELOADED ON OCTOBER 20, 2002
FILE LAST UPDATED ON MARCH 30,2004

FILE COVERS 1771 TO 2003.
*** FILE CONTAINS  8,932,479 SUBSTANCES ***

>>> PLEASE NOTE: Reaction data and substance data are stored in
    separate documents and can not be searched together in one
    query.
    Reaction data for BEILSTEIN compounds may be displayed
    immediately with the display codes PRE (preparations) and REA
    (reactions). A substance answer set retrieved after the search
    for a chemical name, a molecular formula or a structure search
    for example can be restricted to compounds with available
    reaction information by concatenation with PRE/FA, REA/FA or
    more general with RX/FA. The BEILSTEIN Registry Number (BRN)
    is the link between a BEILSTEIN compound and belonging reactions.
    For more detailed reaction searches BRNs can be selected from
    substance answer sets and searched in the next step as reaction
    partner BRNs - Reactant (RX.RBRN) or Product BRN (RX.PBRN).
    After a search for reaction details substance documents
    associated with reactants or products may be retrieved by
    searching RX.PBRNs or RX.RBRNs as BRNs. <<<


>>> FOR SEARCHING PREPARATIONS SEE HELP PRE  <<<

*********************************************************************
* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST.               *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE  *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE         *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.                       *
* FOR PRICE INFORMATION SEE HELP COST                               *
*********************************************************************

=> d his

     (FILE 'HOME' ENTERED AT 15:03:31 ON 12 MAY 2004)

     FILE 'STNGUIDE' ENTERED AT 15:03:51 ON 12 MAY 2004

     FILE 'REGISTRY' ENTERED AT 15:18:24 ON 12 MAY 2004
L1              STRUCTURE UPLOADED
L2            0 S L1
L3           25 S L1 FULL
L4            9 S L3 AND 1/B

     FILE 'CAPLUS' ENTERED AT 15:19:22 ON 12 MAY 2004
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L5             7 S L4

     FILE 'CASREACT' ENTERED AT 15:22:51 ON 12 MAY 2004

     FILE 'CASREACT' ENTERED AT 15:34:05 ON 12 MAY 2004

     FILE 'BEILSTEIN' ENTERED AT 15:36:56 ON 12 MAY 2004

=> s l1 full
FULL SEARCH INITIATED 15:37:06 FILE 'BEILSTEIN'
FULL SCREEN SEARCH COMPLETED -   1495 TO ITERATE

100.0% PROCESSED    1495 ITERATIONS                              0 ANSWERS
SEARCH TIME: 00.00.11

L6             0 SEA SSS FUL L1

=> file gmelin
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                                 0.06     223.74

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)    SINCE FILE      TOTAL
                                                   ENTRY    SESSION
CA SUBSCRIBER PRICE                                 0.00      -6.17

FILE 'GMELIN' ENTERED AT 15:37:24 ON 12 MAY 2004
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FILE LAST UPDATED: 03 MAY 97 - 21 MAY 97      <970503/UP -970521/UP>

>>> CAS REGISTRY NUMBERS FOR 171,499 SUBSTANCES AVAILABLE <<<
>>> FILE CONTAINS 1,070,350 SUBSTANCES <<<
>>> PLEASE NOTE THAT AFTER A SEARCH IN SSTA FIELDS DIS QRD OR
    DIS HIT CAN BE VERY LENGTHY. <<<

**********************************************************************
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR PREDEFINED   *
* FORMATS ARE BASED ON THE SUM OF ALL FIELDS POSSIBLE. THEREFORE;    *
* THESE ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.                  *
* FOR PRICE INFORMATION SEE HELP COST.                               *
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=> s l1 full
FULL SEARCH INITIATED 15:37:30 FILE 'GMELIN'
FULL SCREEN SEARCH COMPLETED -    405 TO ITERATE

100.0% PROCESSED     405 ITERATIONS                              0 ANSWERS
SEARCH TIME: 00.00.05

L7             0 SEA SSS FUL L1

=>

---Logging off of STN---
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